Tetrahydrophthalic anhydride 85-43-8 | DTXSID3026516

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75°	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 251 °C

Global applicability domain: Inside

Local applicability domain index: 4.99e-01

Confidence level: 7.43e-01

Nearest Neighbors from the Training Set

Image not found

Dehydroacetic acid Measured: 270 Predicted: 268

Image not found

2,5-Furandione, 3,4-dimethyl-

Measured: 223 Predicted: 223

Image not found

2,5-Furandione, 3-chloro-

Measured: 196 Predicted: 206

Image not found

Phthalic anhydride Measured: 295 Predicted: 293